SH-STRETCHING INTENSITIES AND INTRAMOLECULAR HYDROGEN BONDING IN ALKANETHIOLS

B. J. MILLER, J. R. LANE, A. H. SODERGREN, H. G. KJAERGAARD, *Department of Chemistry, University of Otago, P.O. Box 56, Dunedin, New Zealand*; M. E. DUNN, AND V. VAIDA, *Department of Chemistry and Biochemistry and CIRES, University of Colorado, Campus Box 215, Boulder, CO 80309*.

The SH-stretching overtone transitions of tert-butylthiol and ethanethiol are observed using FT-IR, NIR and photoacoustic spectroscopies. The intensities of these are compared with OH-stretching overtones from the corresponding alcohols. We explain the paucity of SH-stretching intensity using an anharmonic oscillator local mode model. SH- and OH-stretching overtone spectra of 1,2-ethanedithiol and 2-mercaptoethanol are recorded to observe the different effects that hydrogen bonding involving SH - - - S, SH - - - O and OH - - - S have on the spectra. We discuss these effects with the help of high level ab initio calculations.